

# Metal-Mott Insulator Transition and Spin Exchange of Two-Component Fermi Gas with Spin-Orbit Coupling in Two-Dimension Square Optical Lattices

Beibing Huang\*

Department of Experiment Teaching, Yancheng Institute of Technology, Yancheng, 224051, China  
and Shaolong Wan

Institute for Theoretical Physics and Department of Modern Physics,  
University of Science and Technology of China, Hefei, 230026, China

October 13, 2011

## Abstract

Effects of spin-orbit coupling (SOC) on metal-Mott insulator transition (MMIT) and spin exchange physics (SEP) of two-component Fermi gases in two-dimension half-filling square optical lattices are investigated. In the frame of Kotliar and Ruckenstein slave boson and the second order perturbation theory, the phase boundary of paramagnetic MMIT and spin exchange Hamiltonian are calculated. In addition by adopting two mean-field ansatzs including antiferromagnetic, ferromagnetic and spiral phases, we find that SOC can drive a quantum phase transition from antiferromagnet to spiral phase.

**PACS** number(s): 03.75.Ss, 51.60.+a, 05.70.Fh

## 1 Introduction

In a crystalline solid spin-orbit coupling (SOC), which occurs naturally in systems with broken inversion symmetry and makes the spin degree of freedom respond to its orbital motion, is responsible for many interesting phenomena, such as magnetoelectric effect [1, 2, 3],

---

\*Corresponding author. Electronic address: hbb4236@mail.ustc.edu.cn

visionary Datta-Das spin transistor [4, 5], topological insulator [6, 7] and superconductivity [8, 9]. Taking topological superconductivity for example, it has been predicted to occur in superconductors with a sizable spin-orbit coupling in the presence of an external magnetic field [10, 11, 12, 13, 14]. In these systems the transition to topological phases requires that critical magnetic field is much larger than the superconductivity gap above which an s-wave superconductor is expected to vanish in the absence of SOC. It is SOC that competes with a strong magnetic field to give rise to a topological superconducting phase.

As is known to all that ultracold atom systems can be used to simulate many other systems owing to their many controllable advantages and operabilities [15, 16, 17]. Certainly the simulations to SOC, which are generally equivalent to produce non-abelian gauge potential with optical [18, 19, 20] or radio-frequency fields [21], are also possible and have been realized in a neutral atomic Bose-Einstein condensate (BEC) by dressing two atomic spin states with a pair of lasers [22]. Motivated by such a pioneer experiment and a practical proposal for generating SOC in  $^{40}\text{K}$  atoms [23], BCS-BEC crossover in the two-component Fermi gases with SOC have been widely studied [24, 25, 26, 27, 28, 29, 30, 31].

By contrast in this paper we consider repulsive two-component Fermi gases with SOC in a two-dimensional square optical lattice, and are interested in the effects of SOC on metal-Mott insulator transition (MMIT) and spin exchange physics (SEP) at half filling. Essentially MMIT of two-component Fermi gases without SOC in an optical lattice has been realized experimentally [16] and is driven by the competition between hopping term and on-site interaction in the frame of one-band Hubbard model. When the hopping term dominates, atoms conduct freely in a lattice and the system is a metal. Gradually adjusting on-site interaction to an extent that the gain of the kinetic energy cannot offset the increase of potential energy, on-site interaction forbids the hopping of atoms and the system evolves into Mott insulator (MI). In a MI, SEP is correctly described by quantum antiferromagnetic Heisenberg model, which is known from the famous  $t - J$  model [32] expected to offer a mechanism for high temperature superconductor. Physically this effective antiferromagnetic coupling between the nearest-neighbor spins comes from Pauli exclusion principle and the fact that the hopping of a particle cannot change its spin. Thus to minimize kinetic energy the nearest-neighbor spins must be antiparallel. In the presence of SOC, it has two effects on atom hopping. On the one hand SOC can make atoms move from one site to another site and corresponds to an effective hopping term, so it definitely has important effects on MMIT in view of the above statement. On the other hand, the effective hopping induced by SOC is spin-flipped to support the nearest-neighbor spins parallel. From this viewpoint SOC also dramatically changes SEP. Furthermore it is likely that when the strength of SOC is beyond certain critical value, the system will show a quantum phase transition from antiferromagnetic to other magnetic states.

This paper is organized as follows. In section 2, we firstly derive Hubbard Hamiltonian in two-dimensional square optical lattices with SOC, then by using Kotliar-Ruckenstein (KR) slave bosons [33] we investigate paramagnetic MMIT, i.e. Brinkman-Rice phase transition [34]. In section 3 under the limit of large on-site repulsion and using the second order perturbation theory spin exchange Hamiltonian is obtained. By making mean field approximations we find that the ground state of the system is either antiferromagnetic or spiral depending on the relative magnitude of hopping term and strength of SOC and a quantum phase transition happens between them. The conclusions are given in section 4.

## 2 Metal-MI Phase Transition with SOC

The Hamiltonian of the system we consider is

$$H = \int d^2\vec{r} \left\{ \sum_{\alpha,\beta} \Psi_{\alpha}^{\dagger}(\vec{r}) \left[ \frac{\vec{p}^2}{2m} + V_{OL}(\vec{r}) + \lambda(\sigma_x p_y - \sigma_y p_x) \right] \Psi_{\beta}(\vec{r}) + g \Psi_{\uparrow}^{\dagger}(\vec{r}) \Psi_{\downarrow}^{\dagger}(\vec{r}) \Psi_{\downarrow}(\vec{r}) \Psi_{\uparrow}(\vec{r}) \right\}, \quad (1)$$

where a Fermi atom of mass  $m$  for spin  $\alpha$  is described by the field operators  $\Psi_{\alpha}(\vec{r})$  and  $V_{OL}(\vec{r})$  is optical potential for two-dimensional square lattices.  $\lambda$ ,  $g(>0)$  and  $\vec{\sigma}$  represent the strength of Rashba SOC, two-body contact interaction and Pauli matrix respectively. When temperature is very low and filling factor is not too high, all atoms are constrained into the lowest band of the optical lattice. Expanding the field operator in terms of the Wannier functions  $\Psi_{\alpha}(\vec{r}) = \sum_i a_{i\alpha} w(\vec{r} - \vec{R}_i)$ , where  $a_{i\alpha}$  is the annihilation operator for an atom of spin  $\alpha$  in site  $\vec{R}_i$ , and only retaining on-site interaction and nearest neighbor hopping, we find

$$H = \sum_{\langle i,j \rangle} a_{i\alpha}^{\dagger} t_{ij}^{\alpha\beta} a_{j\beta} + U \sum_i a_{i\uparrow}^{\dagger} a_{i\downarrow}^{\dagger} a_{i\downarrow} a_{i\uparrow}, \quad (2)$$

where the hopping term  $t_{ij}^{\alpha\beta}$  is a  $2 \times 2$  matrix and its elements are  $t_{ij}^{\uparrow\uparrow} = t_{ij}^{\downarrow\downarrow} = -t$ ,  $t_{ij}^{\uparrow\downarrow} = -[t_{ij}^{\downarrow\uparrow}]^* = \Gamma_{i,j}^x - i\Gamma_{i,j}^y$ . These parameters  $t$ ,  $\Gamma_{i,j}^x$ ,  $\Gamma_{i,j}^y$  and  $U$  are related to the Wannier function as follows

$$\begin{aligned} t &= - \int d^2\vec{r} w(\vec{r} - \vec{R}_i) \left[ \frac{\vec{p}^2}{2m} + V_{OL}(\vec{r}) \right] w(\vec{r} - \vec{R}_j), \\ U &= g \int d^2\vec{r} w(\vec{r} - \vec{R}_i) w(\vec{r} - \vec{R}_i) w(\vec{r} - \vec{R}_i) w(\vec{r} - \vec{R}_i), \\ \Gamma_{i,j}^x &= \lambda \int d^2\vec{r} w(\vec{r} - \vec{R}_i) \frac{\partial}{\partial x} w(\vec{r} - \vec{R}_j), \\ \Gamma_{i,j}^y &= \lambda \int d^2\vec{r} w(\vec{r} - \vec{R}_i) \frac{\partial}{\partial y} w(\vec{r} - \vec{R}_j). \end{aligned} \quad (3)$$

From above expressions (3) and the symmetry of Wannier function,  $\Gamma_{i,j}^x$ ,  $\Gamma_{i,j}^y$  satisfy the relations  $\Gamma_{i,j}^x = \Gamma_{j,i}^x = -\Gamma_{j,i}^y = -\Gamma_{i,j}^y$ . Moreover  $\Gamma_{i,j}^x = 0$  if  $i, j$  are nearest neighbor along  $y$  direction and  $\Gamma_{i,j}^y = 0$  if  $i, j$  are nearest neighbor along  $x$  direction. For convenience the parameter  $\Gamma$  is defined  $\Gamma = |\Gamma_{i,j}^x| = |\Gamma_{i,j}^y|$  to represent the strength of SOC.

It is well known that MMIT is a phenomenon of strong correlation. In terms of strong correlation, apart from some numerical methods, such as dynamical mean-field theory [35], a few analytical methods are also available. The first is Gutzwiller variational wave function [36]. In this method to make the calculation tractable, one has to introduce the Gutzwiller approximation which is basically at the mean-field level. Although this method is successful to predict the existence of MMIT, it still has some disadvantages from variational and mean-field approximations. Another method is KR slave bosons [33]. It exactly reproduces the results of Gutzwiller approximation at the saddle-point level and can be improved systematically by considering fluctuations around the saddle point [37]. Hence below we adopt slave bosons to study MMIT with SOC, although our results is at the saddle-point level.

For two-component Fermi gases, the Hilbert space for every lattice site  $i$  consists of four states  $|0\rangle_i$ ,  $|\alpha\rangle_i = a_{i\alpha}^\dagger|0\rangle_i$  and  $|\uparrow, \downarrow\rangle_i = a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger|0\rangle_i$ . In the representation of KR slave bosons, in addition to original fermions, a set of four bosons  $e$ ,  $d$ ,  $p_\alpha$  for every lattice site are introduced so that  $|0\rangle_i = e_i^\dagger|vac\rangle$ ,  $|\alpha\rangle_i = p_{i\alpha}^\dagger a_{i\alpha}^\dagger|vac\rangle_i$  and  $|\uparrow, \downarrow\rangle_i = d_i^\dagger a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger|vac\rangle_i$ , where  $|vac\rangle$  is the vacuum state after introducing slave bosons. It is easily found that  $e_i^\dagger e_i$ ,  $d_i^\dagger d_i$  and  $p_{i\alpha}^\dagger p_{i\alpha}$  represent the projectors on the empty, doubly occupied and singly occupied site. Due to the fact that the introduction of bosons enlarges the Hilbert space of every site to contain some unphysical states, such as  $e_i^\dagger e_i^\dagger|vac\rangle_i$  etc., we must impose three constraints  $e_i^\dagger e_i + p_{i\alpha}^\dagger p_{i\alpha} + d_i^\dagger d_i = 1$ ,  $a_{i\alpha}^\dagger a_{i\alpha} = p_{i\alpha}^\dagger p_{i\alpha} + d_i^\dagger d_i$ . In terms of these bosons and considering above constraints the Hamiltonian (2) is reformulated into

$$H = \sum_{\langle i,j \rangle} a_{i\alpha}^\dagger z_{i\alpha}^\dagger t_{ij}^{\alpha\beta} z_{j\beta} a_{j\beta} + U \sum_i d_i^\dagger d_i, \quad (4)$$

with

$$\begin{aligned} z_{i\alpha} &= (1 - d_i^\dagger d_i - p_{i\alpha}^\dagger p_{i\alpha})^{-1/2} \bar{z}_{i\alpha} (1 - e_i^\dagger e_i - p_{i-\alpha}^\dagger p_{i-\alpha})^{-1/2}, \\ \bar{z}_{i\alpha} &= e_i^\dagger p_{i\alpha} + p_{i-\alpha}^\dagger d_i. \end{aligned} \quad (5)$$

As claimed by KR, the substitution  $z_{i\alpha}$  for  $\bar{z}_{i\alpha}$  ensures  $z_{i\alpha}^\dagger z_{j\beta} = 1$  to recover the results in the limit  $U = 0$  at the saddle-point approximation.

The partition function  $Z$  can be written as a functional integral over the fermion and boson operators

$$Z = \int \mathcal{D}a_\alpha \mathcal{D}e \mathcal{D}p_\alpha \mathcal{D}d \prod_{i\sigma} d\lambda_i^{(1)} d\lambda_{i\alpha}^{(2)} \exp[-\int_0^\beta \mathcal{L}(\tau) d\tau], \quad (6)$$

where the Lagrangian  $\mathcal{L}(\tau)$  is

$$\begin{aligned} \mathcal{L}(\tau) &= \sum_i e_i^\dagger \left[ \frac{\partial}{\partial \tau} + \lambda_i^{(1)} \right] e_i + d_i^\dagger \left[ \frac{\partial}{\partial \tau} + U + \lambda_i^{(1)} - \lambda_{i\uparrow}^{(2)} - \lambda_{i\downarrow}^{(2)} \right] d_i + p_{i\alpha}^\dagger \left[ \frac{\partial}{\partial \tau} + \lambda_i^{(1)} - \lambda_{i\alpha}^{(2)} \right] p_{i\alpha} \\ &+ \sum_{\langle i,j \rangle} a_{i\alpha}^\dagger \left[ \left( \frac{\partial}{\partial \tau} + \lambda_{i\alpha}^{(2)} - \mu \right) \delta_{\alpha\beta} \delta_{ij} + z_{i\alpha}^\dagger t_{ij}^{\alpha\beta} z_{j\beta} \right] a_{j\beta} - \lambda_i^{(1)}, \end{aligned} \quad (7)$$

and  $\mu$ ,  $\lambda_i^{(1)}$ ,  $\lambda_{i\alpha}^{(2)}$  are the chemical potential and Lagrange multipliers, respectively.

Assuming uniform and static boson operators and Lagrange multipliers, i.e. at the saddle point, one can integrate over fermion operators and obtain for thermodynamic potential of single site

$$\Omega = \lambda^{(1)}(e^2 + d^2 + p_\alpha^2 - 1) + U d^2 - \lambda_\alpha^{(2)}(d^2 + p_\alpha^2) - \frac{1}{\beta N} \sum_{k\alpha} \ln[1 + e^{-\beta E_{k\alpha}}] \quad (8)$$

with  $E_{k\alpha} = [\epsilon_{k\uparrow} + \epsilon_{k\downarrow} + \alpha \sqrt{(\epsilon_{k\uparrow} - \epsilon_{k\downarrow})^2 + 4z_\uparrow^2 z_\downarrow^2 \Gamma_k^2}] / 2$ ,  $\epsilon_{k\alpha} = \epsilon_k z_\alpha^2 - \mu + \lambda_\alpha^{(2)}$ ,  $\epsilon_k = -2t(\cos k_x a + \cos k_y a)$ ,  $\Gamma_k = 2\Gamma \sqrt{\sin^2 k_x a + \sin^2 k_y a}$ . It is to be noted that  $a$ ,  $N$  are lattice length and the number of lattice site, and wavevector  $k$  belongs to two dimensional Brillouin zone. At

this time the seven parameters  $e$ ,  $p_\alpha$ ,  $d$ ,  $\lambda^{(1)}$  and  $\lambda_\alpha^{(2)}$  are obtained by minimizing  $\Omega$ , and the chemical potential at half filling by thermodynamic relation  $-\frac{\partial\Omega}{\partial\mu} = 1$ . These equations are called saddle-point and number equations.

From  $\frac{\partial\Omega}{\partial\lambda^{(1)}} = \frac{\partial\Omega}{\partial\lambda_\alpha^{(2)}} = 0$  and  $-\frac{\partial\Omega}{\partial\mu} = 1$ , one can get  $e^2 = d^2$ . Supposing paramagnetic solution  $p_\uparrow^2 = p_\downarrow^2$ , then  $p^2 = \frac{1}{2} - d^2$ ,  $z_\uparrow^2 = z_\downarrow^2 = z^2 = 8d^2(1 - 2d^2)$ . According to  $\frac{\partial\Omega}{\partial p_\alpha} = \frac{\partial\Omega}{\partial e} = \frac{\partial\Omega}{\partial d} = 0$ ,  $\lambda_\uparrow^{(2)} = \lambda_\downarrow^{(2)} = \frac{U}{2}$ ,  $\epsilon_{k\uparrow} = \epsilon_{k\downarrow}$ ,  $E_{k\alpha} = [\epsilon_k + \alpha\Gamma_k]z^2 - \mu + \frac{U}{2}$ ,  $\lambda^{(1)} = \frac{U}{2} - 16\xi d^2(3 - 4d^2)$  with

$$\xi = \frac{1}{N} \sum_k \left[ \frac{\epsilon_k + \Gamma_k}{e^{\beta E_{k\uparrow}} + 1} + \frac{\epsilon_k - \Gamma_k}{e^{\beta E_{k\downarrow}} + 1} \right]. \quad (9)$$

Substituting above relations into saddle-point and number equations, one still has two equations satisfied by  $\mu$  and  $d$

$$\begin{aligned} \frac{1}{N} \sum_k \left[ \frac{1}{e^{\beta E_{k\uparrow}} + 1} + \frac{1}{e^{\beta E_{k\downarrow}} + 1} \right] &= 1, \\ U + 8\xi(1 - 4d^2) &= 0. \end{aligned} \quad (10)$$

At zero temperature, in the frame of KR slave bosons,  $d^2 = 0$  corresponds to the vanishing of the number of doubly occupied sites and indicates that the system is undergoing a MMIT. From this criterion one has numerically solved the equations (10). The numerical results suggest the chemical potential is still fixed at  $\mu = U/2$ . Hence at zero temperature

$$\xi = \frac{1}{N} \sum_k \{ (\epsilon_k + \Gamma_k)\Theta[-(\epsilon_k + \Gamma_k)] + (\epsilon_k - \Gamma_k)\Theta[-(\epsilon_k - \Gamma_k)] \}. \quad (11)$$

and the phase boundary of MMIT is

$$U = -8\xi, \quad (12)$$

where  $\Theta(x)$  is Heaviside step function. Without SOC,  $\xi = \frac{2}{N} \sum_k \epsilon_k \Theta[-\epsilon_k]$  and the phase boundary (12) is the same as the result in [33]. In Fig.1 the phase boundary of MMIT is shown. From Fig.1, very explicitly SOC stabilizes the MI, which is consistent with the fact that SOC can be regarded as an effective hopping term. Besides instead of adjusting  $t$  MMIT can also be driven by changing SOC, so one has found another way to realize the MMIT.

### 3 Spin Exchange and Magnetic Phase Transition with SOC

As demonstrated in the section 2, at half filling when  $U \gg t$  and  $U \gg \Gamma$ , the hopping of atoms are forbidden and the system evolves into MI with spin  $S = \frac{1}{2}$  for every lattice site. In the MI we could regard  $t$  and  $\Gamma$  as perturbations. In the limit of  $t = \Gamma = 0$  the energy of the system does not depend on the spin orientations on different sites. When  $t, \Gamma$  are finite but small, we expect that we still have spin  $S = \frac{1}{2}$  in each site, but atom hopping processes induce effective interactions between these spins, usually called spin exchange interaction [38]. To construct an effective spin exchange Hamiltonian for this system, we note that

in the second order in  $t$ ,  $\Gamma$  it can be written as a sum of interaction terms for all nearest neighbor sites. These pairwise interactions can be found by solving a two-site problem in the second order in  $t$ ,  $\Gamma$ .

The ground state manifold for two-site problem with one atom in each site composes of four degenerate zero-energy states

$$\begin{aligned} |1\rangle &= |\uparrow\rangle_i |\uparrow\rangle_j, |2\rangle = |\uparrow\rangle_i |\downarrow\rangle_j, \\ |3\rangle &= |\downarrow\rangle_i |\uparrow\rangle_j, |4\rangle = |\downarrow\rangle_i |\downarrow\rangle_j, \end{aligned} \quad (13)$$

with  $i, j$  labelling two sites. The first order perturbation theory takes us out of the ground state manifold and can be neglected. In the second order atom hoppings can connect all four states by two intermediate states  $|5\rangle = |\uparrow, \downarrow\rangle_i |0\rangle_j$  and  $|6\rangle = |0\rangle_i |\uparrow, \downarrow\rangle_j$ . To find spin exchange Hamiltonian we need calculate all matrix elements [38]

$$M_{ab} = \sum_c \frac{\langle a | H_k | c \rangle \langle c | H_k | b \rangle}{E_b^0 - E_c^0}, \quad (14)$$

where states  $|a\rangle, |b\rangle$  and  $|c\rangle$  respectively belong to ground state manifold and intermediate states with  $E^0$  representing eigenenergy of corresponding state in the zeroth order. The calculation is very direct and when  $i, j$  are nearest neighbor along  $x$  direction, we have  $M_{11} = M_{14} = M_{41} = M_{44} = \frac{2\Gamma_{ij}^x \Gamma_{ji}^x}{U}$ ,  $M_{12} = M_{21} = M_{24} = M_{42} = \frac{2t\Gamma_{ij}^x}{U}$ ,  $M_{13} = M_{31} = M_{34} = M_{43} = \frac{2t\Gamma_{ij}^x}{U}$ ,  $M_{22} = -M_{23} = -M_{32} = M_{33} = -\frac{2t^2}{U}$ . According to spectral representation of an operator, magnetic Hamiltonian of two-site problem is  $H_{i,j} = \sum_{a,b} |a\rangle M_{ab} \langle b|$ . Making substitutions  $|1\rangle \rightarrow a_{i\uparrow}^\dagger a_{j\uparrow}^\dagger$ ,  $|2\rangle \rightarrow a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger$ ,  $|3\rangle \rightarrow a_{i\downarrow}^\dagger a_{j\uparrow}^\dagger$ ,  $|4\rangle \rightarrow a_{i\downarrow}^\dagger a_{j\downarrow}^\dagger$  and using algebra of spin operator  $\vec{S}_i = \frac{1}{2} a_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} a_{i\beta}$ , we get

$$H_{i,j} = \frac{4t^2}{U} \vec{S}_i \cdot \vec{S}_j + \frac{8t\Gamma_{ij}^x}{U} (S_{ix} S_{jz} - S_{iz} S_{jx}) + \frac{4\Gamma_{ij}^x \Gamma_{ji}^x}{U} (S_{iz} S_{jz} + S_{ix} S_{jx} - S_{iy} S_{jy}). \quad (15)$$

By the same procedure, when  $i, j$  are nearest neighbor along  $y$  direction we get

$$H_{i,j} = \frac{4t^2}{U} \vec{S}_i \cdot \vec{S}_j + \frac{8t\Gamma_{ij}^y}{U} (S_{iy} S_{jz} - S_{iz} S_{jy}) + \frac{4\Gamma_{ij}^y \Gamma_{ji}^y}{U} (S_{iz} S_{jz} + S_{iy} S_{jy} - S_{ix} S_{jx}). \quad (16)$$

Thus spin exchange Hamiltonian of the whole system is

$$H_{se} = \sum_{\langle i,j \rangle} H_{i,j}. \quad (17)$$

Some comments about (17) is following. If  $\Gamma = 0$   $H_{se}$  describes isotropic quantum antiferromagnet, consistent with  $t - J$  model. When  $\Gamma \neq 0$ , main effect of SOC is to break spin conservation by two ways, one of which, corresponding to the second term in (15) and (16), flips one spin of two nearest neighbor sites, while the other flips simultaneously two spins corresponding to the third term in (15) and (16). Thus the antiferromagnetic state will be unstable when the strength of SOC  $\Gamma$  is beyond certain critical value.

Now we decide the ground state of the system at mean-field level. This corresponds to regard quantum spin operator  $\vec{S}_i$  as a classical vector. The first mean-field ansatz including

ferromagnetic and antiferromagnetic states is that spin configurations in two sublattices of a square lattice take different values specified respectively by coordinate angle  $(\vartheta, \varphi)$  and  $(\gamma, \delta)$  with  $0 \leq \vartheta, \gamma < \pi$  and  $0 \leq \varphi, \delta < 2\pi$ , the mean-field energy scaled by  $U$  is

$$E = 8N^2 \left[ (\tilde{t}^2 - \tilde{\Gamma}^2) \cos \vartheta \cos \gamma + \tilde{t}^2 \sin \vartheta \sin \gamma \cos(\varphi - \delta) \right], \quad (18)$$

where a  $2N \times 2N$  lattice is assumed and  $\tilde{t} = t/U$ ,  $\tilde{\Gamma} = \Gamma/U$ . Easily found that energy only depends on the difference of  $\varphi$  and  $\delta$ , for convenience we can choose  $\delta = 0$ . Owing to factor  $\sin \vartheta \sin \gamma \geq 0$ , the minimization of energy leads to  $\varphi = \pi$ . Minimizing energy about  $\vartheta, \gamma$ , we get

$$\begin{aligned} (\tilde{t}^2 - \tilde{\Gamma}^2) \sin \vartheta \cos \gamma + \tilde{t}^2 \cos \vartheta \sin \gamma &= 0, \\ (\tilde{t}^2 - \tilde{\Gamma}^2) \cos \vartheta \sin \gamma + \tilde{t}^2 \sin \vartheta \cos \gamma &= 0. \end{aligned} \quad (19)$$

Equations (19) have two sets of solution  $\vartheta = \gamma = 0$  and  $\vartheta = \gamma = \pi/2$ . The first solution corresponds to ferromagnet along  $z$  direction with  $E_{FE} = 8N^2(\tilde{t}^2 - \tilde{\Gamma}^2)$  and the second corresponds to antiferromagnet along  $x$  direction with  $E_{AF} = -8N^2\tilde{t}^2$ . If  $E_{FE} < E_{AF}$  ground state is ferromagnetic, on the contrary ground state is antiferromagnetic. Thus this mean-field ansatz predicts a phase transition from antiferromagnet to ferromagnet and the critical point is  $E_{FE} = E_{AF}$ , i.e.  $\tilde{\Gamma} = \sqrt{2}\tilde{t}$ .

The motivation of the second mean-field ansatz comes from  $t = 0$  limit in spin exchange Hamiltonian (17). Letting  $t = 0$  the classical spin configuration minimizing energy satisfies three conditions: (1)  $z$  components of all spins are equal; (2) for a random chain along  $x$  direction  $x$  components of all spins are equal but  $y$  component must be alternating; (3) for a random chain along  $y$  direction  $y$  components of all spins are equal but  $x$  component must be alternating. Such spin configuration, which we call spiral phase and shown in Fig.2, is permissible in a square lattice. From above three conditions if coordinate angle  $(\theta, \phi)$  of a spin in the lattice is specified, energy of the system is

$$E_{SP} = 8N^2(\tilde{t}^2 \cos^2 \theta - \tilde{\Gamma}^2), \quad (20)$$

and its minimization gives rise to  $\theta = \pi/2$ ,  $E_{SP} = -8N^2\tilde{\Gamma}^2$ . Comparing  $E_{SP}$  with  $E_{FE}$  we find that the ferromagnetic state is always a metastable state. As a result phase transition predicted by the first mean-field ansatz does not exist, we get a phase transition from antiferromagnet to spiral phase with critical point  $\tilde{\Gamma} = \tilde{t}$ . Fig.1 also shows magnetic phase diagram in terms of such two mean-field ansatzs. Physically the metastability of ferromagnetic state is attributed to the fact that SOC breaks spin conservation.

## 4 Conclusions

In conclusion we have discussed MMIT and SEP of two-component Fermi gases with SOC in two-dimensional half-filling square optical lattices in the frame of KR slave bosons and second-order perturbation theory. Comparing with the case without SOC, SOC not only enlarges the region of MI in the phase diagram and introduces another way to realize MMIT, but also dramatically affects SEP due to SOC breaking spin conservation. Importantly by adopting two mean-field ansatzs we find that SOC can drive a phase transition from

antiferromagnet to spiral phase. Experimentally this phase transition can be observed by either adjusting optical lattices to suppress the hopping term or decreasing the strength of SOC.

## Acknowledgement

The work was supported by National Natural Science Foundation of China under Grant No. 10675108. The author Huang also thanks Foundation of Yancheng Institute of Technology under Grant No. XKR2010007.

## References

- [1] I. E. Dzyaloshinskii, Sov. Phys. JETP 10, 628 (1959).
- [2] Y. Kato, R. C. Myers, A. C. Gossard and D. D. Awschalom, Phys. Rev. Lett. 93, 176601 (2004).
- [3] S. D. Ganichev, S. N. Danilov, P. Scheider, V. V. Belkov, L. E. Golub, W. Wegscheider, D. Weiss and W. Prettl, arXiv:0403641.
- [4] S. Datta and B. Das, Appl. Phys. Lett. 56, 665 (1990).
- [5] J. Schliemann, J. C. Egues and D. Loss, Phys. Rev. Lett. 90, 146801 (2003).
- [6] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
- [7] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
- [8] A. P. Schnyder, S. Ryu, A. Furusaki and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
- [9] S. Tewari, T. D. Stanescu, J. D. Sau and S. D. Sarma, New J. Phys. 13, 065004 (2011).
- [10] J. D. Sau, R. M. Lutchyn, S. Tewari and S. Das Sarma, Phys. Rev. Lett. 104, 040502 (2010).
- [11] S. Tewari, J. D. Sau and S. Das Sarma, Ann. Phys. 325, 219 (2010).
- [12] J. D. Sau, S. Tewari, R. Lutchyn, T. Stanescu and S. Das Sarma, Phys. Rev. B 82, 214509 (2010).
- [13] P. Ghosh, J. D. Sau, S. Tewari and S. Das Sarma, Phys. Rev. B 82, 184525 (2010).
- [14] M. Sato and S. Fujimoto, Phys. Rev. B 82, 134521 (2010).
- [15] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch and I. Bloch, Nature (London) 415, 39 (2002).
- [16] R. Jördens, N. Strohmaier, K. Günter, H. Moritz and T. Esslinger, Nature (London) 455, 204 (2008).



- [17] M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen and U. Sen, *Adv. Phys.* 56, 243 (2007).
- [18] K. Osterloh, M. Baig, L. Santos, P. Zoller and M. Lewenstein, *Phys. Rev. Lett.* 95, 010403 (2005).
- [19] J. Ruseckas, G. Juzeliunas, P. Ohberg and M. Fleischhauer, *Phys. Rev. Lett.* 95, 010404 (2005).
- [20] X.-J. Liu, M. F. Borunda, X. Liu and J. Sinova, *Phys. Rev. Lett.*, 102, 046402 (2009).
- [21] N. Goldman, I. Satija, P. Nikolic, A. Bermudez, M. A. Martin-Delgado, M. Lewenstein and I. B. Spielman, *Phys. Rev. Lett.*, 105, 255302 (2010).
- [22] Y.-J. Lin, K. J.-Garca and I. B. Spielman, *Nature (London)* 471, 83 (2011).
- [23] J. D. Sau, Rajdeep Sensarma, Stephen Powell, I. B. Spielman and S. Das Sarma, *Phys. Rev. B* 83, 140510 (2011).
- [24] H. Hu, L. Jiang, X.-J. Liu and H. Pu, *arXiv:1105.2488* (2011).
- [25] Z.-Q. Yu and H. Zhai, *arXiv:1105.2250* (2011).
- [26] J. P. Vyasankere, S. Zhang and V. B. Shenoy, *arXiv:1104.5633* (2011).
- [27] J. P. Vyasankere and V. B. Shenoy, *arXiv:1108.4872* (2011).
- [28] L. Han and C. A. R. Sá de Melo, *arXiv:1106.3613* (2011).
- [29] G. Chen, M. Gong and C. Zhang, *arXiv:1107.2627* (2011).
- [30] M. Iskin and A. L. Subasi, *arXiv:1106.0473* (2011).
- [31] K. Seo, L. Han and C. A. R. Sá de Melo, *arXiv:1108.4068* (2011).
- [32] P. W. Anderson, *Science* 235, 1196 (1987).
- [33] G. Kotliar and A. E. Ruckenstein, *Phys. Rev. Lett.* 57, 1362 (1986).
- [34] W. F. Brinkman and T. M. Rice, *Phys. Rev. B* 2, 4302(1970).
- [35] A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, *Rev. Mod. Phys.* 68, 13 (1996).
- [36] M. C. Gutzwiller, *Phys. Rev. Lett.* 10, 159 (1963); *Phys. Rev.* 134, A923 (1964); 137, A1762 (1965).
- [37] M. Lavagna, *Phys. Rev. B* 41, 142 (1990).
- [38] A. Imambekov, M. Lukin and E. Demler, *Phys. Rev. A* 68, 063602 (2004).

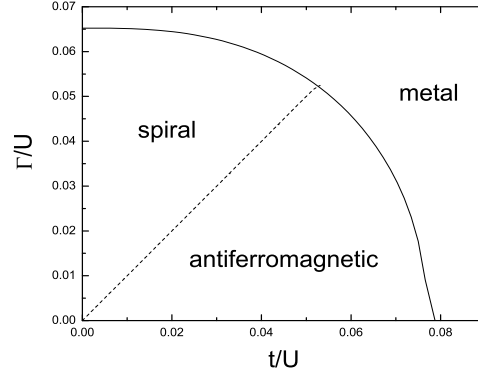


Figure 1: The phase diagram of a repulsively interacting two-component Fermi gas with spin-orbit coupling in a square optical lattice. The solid line is the phase boundary of metal-Mott insulator transition, while the dashed line is one of antiferromagnetic-spiral phases.

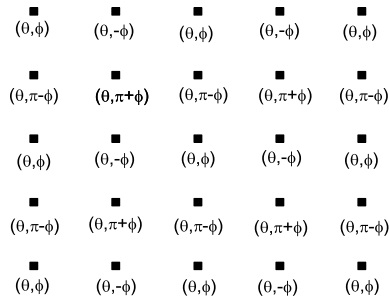


Figure 2: Spin configuration of spiral phase is shown with small squares representing lattice sites.  $(\theta, \phi)$ ,  $(\theta, -\phi)$ ,  $(\theta, \pi - \phi)$  and  $(\theta, \pi + \phi)$  are coordinate angles of spins.